Indian J. Phys. **49**, 631-634 (1975)

Phonon dispersion and electrical resistivity of Potassium

SUNIL KUMAR AND S. TOLPADI

Department of Physics, Indian Institute of Technology, Kharagpur, West Bengal

(*Received* 4 *March*, 1975)

Very recently a number of lattice dynamical studies of alkali metals have been reported (see for example Jogi 1974; Prakash *et al* 1974) using electron gas angular force model. Invariably these studies include electron-ion interaction on the basis of Sharma & Joshi (1963) formalism. Lax (1965) has criticized the approach of Sharma & Joshi 1963) since it lacks the symmetry requirements of the crystal lattice In other words their computed frequencies are not periodic in the reciprocal space. This led Shukla *et al* (1973) to study copper by including the electron-ion interaction through Krebs (1964) model. Cochran (1965) pointed out that such an approach is also defective in the sense that it does not fulfill the internal force equilibrium condition of the lattice. The derivative of long-range screened Coulomb interaction energy in Krebs model (1964) does not vanish in equilibrium configuration. Therefore all these studies (Jogi 1974, Prakash *et al* 1974; Shukla *et al* 1973) require modifications

In the present paper we develop a model for b c c metals which does not suffer from any of the drawbacks discussed above. Angular forces out to second neighbours are considered on the basis of Clark *et al* (1964) model. Electron-ion interactions are considered through a linearized Thomas-Fermi theory for the whole crystal (Cheveau 1968). We report herein the lattice dynamical calculations on the dispersion curves and the electrical resistivity of potassium.

The secular determinant used to determine the phonon frequencies ω is given by

$$|D(q)-m\omega^2 I| = 0, \qquad \ldots (1)$$

where m is ionic mass, I is unit matrix and $D(q)$ is dynamical matrix. Proceeding in the usual manner the elements of the dynamical matrix $D_{ij}(q)$ is split into an ion-ion interaction $D_{ij}^{i-i}(q)$ and electron-ion interaction term $D_{ij}^{e-i}(q)$. The explicit expressions for the various elements of dynamical matrix are given by

$$D_{ii}^{i-i}(q) = 6(A_1+2B_1+3B_2)(1-C_1C_2C_3)+4(A_2+4B_1)S_1^2+2(3B_2-2B_1)(S_2^2+S_3^2) \qquad \ldots (2)$$

$$D_{ij}^{i-i}(q) = 8(A_1-B_1+\tfrac{3}{2}B_2)S_1S_2C_3 \qquad \ldots (3)$$

$$D_{ij}^{e-i}(q) = \frac{a^3\lambda^2(0)K_e}{4}\sum_G\left[\frac{(q+G)_i(q+G)_j}{|q+G|^2+\lambda^2(L_1)} - \frac{G_jG_i}{|G|^2+\lambda^2(L_2)}\right], \quad \ldots (4)$$

where $L_1 = |q+G|/(2k_F)$, $L_2 = |G|/(2k_F)$ and $\lambda(L)$ is the Thomas-Fermi screening parameter as modified by Langer & Vosko (1959); A_1 and A_2 are constants associated with the central forces between nearest and next nearest neighbours respectively, B_1 and B_2 are the corresponding angular force constants and other symbols have their usual meaning.

For a lattice of cubic symmetry the electrical resistivity ρ due to phonon scattering within free electron approximation is given by

$$\rho = \frac{3\hbar}{4\pi K_B e^2 v_F^2 k_F^3 mNT}\sum_p \int d\Omega \int \frac{K^2(1-u^2)^{\frac{1}{2}}(K.e_{qp})^2 C^2(K)}{\{\exp(\beta\omega_{qp})-1\}\{1-\exp(-\beta\omega_{qp})\}}\,dK, \quad \ldots (5)$$

where $u = \frac{K}{2k_F}$, $\beta = \frac{\hbar}{K_BT}$, e is electronic charge, K_B is the Boltzman constant, N is the number of unit cells per unit volume T is the absolute temperature, ω_{qp} and e_{qp} are the angular frequency and polarization vector respectively for phonon wave vector q and mode of vibration P, v_F is the velocity of electron and, K is the scattering vector $C(K)$ are Bardeen (1937) matrix elements and for free electron,

$$C(K) = \frac{[V(r)-E]K^2+W(K)q_s^2}{q_s^2+K^2}\,G(q\,r), \quad \ldots (6)$$

$E-V(r)$ is kinetic energy of an electron in the lowest state at the surface of atomic polyhedron of radius r and $q_s^2 = 4\pi ne^2/W(K)$ n is electron density and

$$W(K) = \tfrac{3}{8}E_F\left(\tfrac{1}{2}+\frac{4k_F^2-K^2}{8k_FK}\ln\left|\frac{2k_F+K}{2k_F-K}\right|\right)^{-1}. \quad \ldots (7)$$

The Bardeen interference factor is given by $G(x) = 3(\sin x - x\cos x)/x^3$.

We apply the above formulation to potassium. To evaluate all the five model parameters use has been made of three exprerimental elastic constants (Marquardt *et al* 1965) and two phonon frequencies from the Brillouin zone boundary (Cowley *et al* 1966) The numerical values of the force constants are $A_1 = 1.2988$, $A_2 = 0\,6454$, $B_1 = 0.0395$, $B_2 = -0.1887$, $aK = -0.2692$ all in units of 10^3 dyn cm.$^{-1}$. The phonon frequencies have been determined from the solution of secular eq. (1) using these values of force constants. The calculation of the temperature variation of the electrical resistivity of potassium has been made from eq. (5). The integration over K has been performed numerically while the integration over the solid angle Ω has been carried out with the help of six term approximation as developed by Betts *et al* (1956). While integrating over K the contribution of the normal and Umklapp processes to the total resistivity

was evaluated separately. A distribution between these two processes was made in a realistic manner (Pal 1973). For the Normal process the scattering vector $K = q$, where q lies in the first Brillouin zone. For Umklapp process $K = q + G$, where K goes beyond the Brillouin zone but q is constrained to lie in it. The minimum value of K, at which U process begins can be obtained from the knowledge of reciprocal lattice vector of b c c. structures. Algorithm developed for numerical computation was simulated on IBM 360/44 computer system.

The theoretically calculated phonon dispersion curves of potassium together with the 9°K neutron spectrometry data of Cowley *et al* (1968) are plotted in figure 1(a). In order to show a definite importance of the present modification in electron-ion interaction term, we have also plotted in figure 1(a) the model calculations of Prakash *et al* (1974). It is seen that the present theoretical dis-

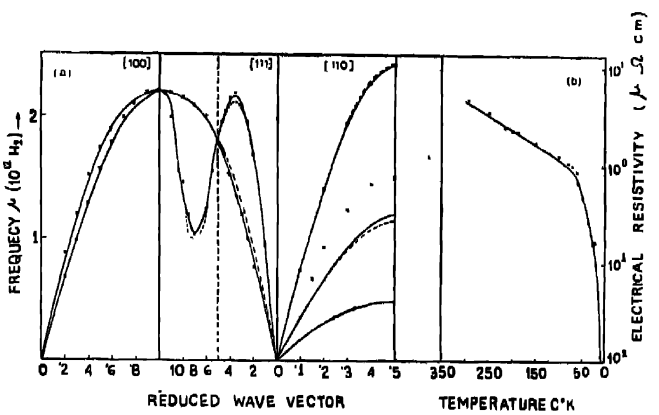

Figure 1(a) Dispersion curves for potassium along the three symmetry directions. Solid lines correspond the present model calculations while broken curves are based on the calculations of Prakash *et al* (1974). Experimental points (Cowley *et al* 1966) are indicated by O, ×.

(b) The temperature variation of the electrical resistivity of potassium. Experimental points of MacDonald *et al* (1956) × and Dugdale *et al* (1962) O

persion curves give much better description of experimental neutron scattering data compared to the dispersion curves of Prakash *et al* (1974) which is a significant achievement of our model. However, this modification is justified by the metallic character of the solid. The computed results of the electrical resistivity of potassium are presented in figure 1(b) along with the experimental data of MacDonald *et al* (1956) and Dugdale *et al* (1962) for comparison. A systematic increase in the U-contribution to the resistivity was observed with temperature. The U-process resistivity reaches a maximum value around 10°K, its contribution at this temperature being about 60% of total resistivity. At 300°K its contribution drops down to about 50%. It can be seen that theoretical values of electrical resistivity are in reasonable agreement with the experimental data.

The discrepancy between theory and experiment is attributed to the use of Bardeen formula which ignores exchanges and correlation effects. Another source of discrepancy is the neglect of temperatuere dependence of elastic constants and other anharmonic effects.

It is concluded that the model proposed here satisfies the symmetry properties and preserves internal force equilibrium of the lattice without recourse to any external forces. This new model gives very good description of dispersion curves and reveals that the contribution of electron-ion interaction is quite significant Such a model when coupled with Bardeen model of electron scattering gives reasonable descriptions of electrical resistivity. In view of actual physical interaction incorporated in the present study our model should therefore be considered more meaningful than the existing models which are generally used in the lattice dynamical studies of b c.c. metals A detailed report with application to other metals is in preparation.

References

Bardeen J. 1937 *Phys. Rev.* **52**, 688.
Betts D D., Bhatia A B. & Wyman M. 1956 *Phys Rev* **104**, 37.
Cheveau L. 1968 *Phys Rev.* **169**, 496.
Clark B. C., Gazis D. C & Wallis R. F. 1964 *Phys. Rev* **134A**, 1486
Cochran W. 1965 *Lattice dynamics* ed R. F. Wallis (Oxford Pergamon Press).
Cowley R A , Woods A. D. B. & Dolling G. 1966 *Phys. Rev.* **150**, 487
Dugdale J S. & Fugan D. 1962 *Proc. R Soc.* **A270**. 186.
Jogi S 1974 *J Phys. F. Metal Phys.* **4**. 11
Krebs K. 1964 *Phys. Lett.* **10**, 12.
Langer J. S & Vosko S H. 1950 *J. Chem. Phys. Solids* **12**, 196.
Lax M 1965 *Lattice Dynamics* ed R. F. Wallis (Oxford Pergamon Press), p. 179.
MacDonald D K. C., White G. K & Woods S. P 1956 *Proc. R. Soc.* **A235**, 358.
Marquardt W. R. & Trivisonno J. 1965 *J. Phys. Chem. Solids* **26**, 273.
Pal S. 1973 *J Phys. F. Metal Phys* **3**, 1296
Prakash J , Pathak L. P. & Hemkar M P. 1974 *J. Phys. F. Metal Physics* **4**, 1107.
Sharma P K. & Joshi S. K. 1963 *J. Chem. Phys.* **39**, 2633.
Shukla M. M. & Closs H. 1973 *J. Phys. F. Metal Phys.* **3**, L83.